WE CLAIM:

1. A crystal of IMPDH isolated from a bacterial preparation.

2. The crystal of claim 1 further characterized by ability to provide x-ray diffraction patterns useful to define molecular structures for bacterial IMPDH enzymes.

3. The crystal of claim 1 wherein the bacterial preparation is a pure culture of *Streptococcus pyogenes*.

4. A method for developing lead compounds for an inhibitor of bacterial IMPDH, said method comprising

a. obtaining a crystal of bacterial IMPDH;

b. recording x-ray diffraction data from said crystal; and

c. using said diffraction data to generate an electron density map consistent with the model for the molecular structure of IMPDH.

5. A molecule or molecular complex comprising an IMPDH binding pocket defined by the structural coordinates of IMPDH amino acids 50-56, 75-80, 229-235, 252-260, 283-286, 302-322, 343-345, 365-433, and 449-455 according to Table 7 or a homologue of said molecule or molecular complex.

6. A molecule or molecular complex comprising all or any parts of a binding pocket defined by structure coordinates of IMPDH amino acids, according to Table 7, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has an amino acid sequence identity of 60% or greater relative to the *S. pyogenes* IMPDH binding pocket.

7. A molecule comprising coordinates from *S. pyogenes* IMPDH amino acids 50-56, 75-80, 229-235, 252-260, 283-286, 302-322, 343-345, 365-433, and 449-455 .

8. A crystalline IMPDH molecule having IMP in its binding site.

9. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex comprising all or any parts of a binding pocket defined by structure coordinates of IMPDH amino acids, according to Table 7, or a homologue of said molecule or molecular complex,

wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.9.

10. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine-readable data, using a machine programmed with instructions for using said first set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine-readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates for IMPDH according to Table 7; and said second set of data comprises an x-ray diffraction pattern of a molecule or molecular complex of unknown structure.

11. A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex comprising the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and a binding pocket of the molecule or molecular complex; and

b. analyzing the results of said fitting operation to quantify the association between the chemical entity and the binding pocket.

12. A method of utilizing molecular replacement to obtain structural information about a molecule or a molecular complex of unknown structure by using the structure coordinates set forth in Table 7, said method comprising the steps of:

a. crystallizing said molecule or molecular complex;

b. generating the x-ray diffraction pattern from said crystallized molecule or molecular complex;

c. applying at least a portion of the structure coordinates set forth in Table 7 to the x-ray diffraction pattern to generate a three-dimensional electron density map of at least a portion of the molecule or molecular complex whose structure is unknown.

13. The method according to claim 12, wherein the molecule or molecular complex comprises a polypeptide selected from an IMPDH homologue.

14. A method for preparing a IMPDH/IMP crystal comprising the steps of

a. forming a complex between IMPDH and IMP;

b. monitoring the accumulation of the IMPDH/IMP complex; and

c. crystallizing the complex formed in step a.